
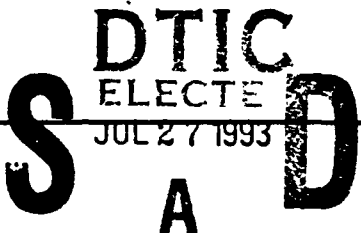


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**FINAL REPORT  
PARALLEL PROCESSING AND SCIENTIFIC APPLICATIONS**

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**Summary**

With three years of AFOSR support we have completed several major projects in the area of parallel processing. Farhat has led efforts in aerospace engineering, especially in the implementation of structural computations on MPP systems. McBryan has led efforts in the area of performance evaluation and in the application of MPP systems to fluid dynamical applications. A total of 81 papers were written describing, and acknowledging, AFOSR supported research. These are listed in sections A.4, B.4, C.1.1 and C.2.3. Six graduate students and three postdoctoral researchers were supported under the grant.

The report will be organized along the lines of the two principal research efforts: MPP applications and MPP performance evaluation.

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## **A. COMPUTATIONAL STRUCTURAL MECHANICS ON ADVANCED ARCHITECTURES**

C. Farhat

### **A.1 RESEARCH OBJECTIVES AND STATEMENT OF WORK**

The growing interest in sophisticated structures such as next generation composite aircraft, space stations, ceramics engines and high performance armors, places increasing demands on the optimality of the structural components used. These demands are met by improving both the accuracy and efficiency of the computational tools used to develop and analyze these structures. The computational demands of these structures are so great, that engineers must frequently be satisfied with rather crude linear analysis even though the large deformations involved demand nonlinear analysis in order to properly represent the structural behavior. Moreover, the realistic simulation of the nonlinear dynamics of these systems remains beyond the feasible range of the current vector super-computers. The true potential for execution improvement lies in parallel and massively parallel computing.

Even though today supercomputers are routinely used by large industrial corporations, parallel processors are thought of as exotic machines. Currently, only a fraction of the engineering community is engaged in applying the concurrent computation technology. Incorporation of these new machines in the mainstream of large scale computations is more challenging than that of supercomputers, and will have a greater impact on computational engineering power. Moving engineering applications to concurrent processors faces significant obstacles that will have to be resolved as such machines are becoming available on a commercial scale. These obstacles center on: (a) methods, (b) algorithms, and (c) software. The present proposal addresses all of these issues. More specifically, the objectives of this research are: (a) to investigate, (b) implement, and (c) evaluate tools for concurrent processing of very large structural engineering problems.

The word tool is used in a broad sense. It includes methods, algorithms, and software.

## **A.2 ACCOMPLISHMENTS**

### **A.2.1 The FETI Method.**

The Finite Element Tearing and Interconnecting (FETI) method initially developed under this grant is a practical and efficient domain decomposition (DD) method for the parallel solution of self-adjoint elliptic partial differential equations.

A given spatial domain is partitioned into non-overlapping subdomains where an incomplete solution for the primary field is first evaluated using a direct solver.

Next, intersubdomain field continuity is enforced via Lagrange multipliers applied at the subdomain interfaces. This "gluing" phase generates a smaller size symmetric dual problem where the unknowns are the Lagrange multipliers, and which is best solved with a preconditioned conjugate gradient (PCG) algorithm. Each iteration of the PCG algorithm requires the solution of independent subdomain problems. For static structural analysis, every floating subdomain is associated with a singular stiffness matrix and generates a set of interface constraints. Consequently, the system of equations governing the dual interface problem is in general indefinite. The FETI algorithm deals with both issues by incorporating in the solution the contribution of the subdomain rigid body modes and by solving the indefinite interface problem with a preconditioned conjugate projected gradient algorithm (PCPG). Each projection step in the PCPG algorithm leads to a "natural" coarse problem. We have shown that the FETI method with the Dirichlet preconditioner is asymptotically optimal --- that is, the condition number of the preconditioned dual interface problem is independent of the number of subdomains and grows only slowly when the mesh size  $h$  approaches 0. Therefore, the FETI method is scalable to Massively Parallel Processors (MPP).

We have applied the FETI method to the solution of three-dimensional structural problems discretized essentially with beam and shell elements. For such problems, we have shown that the FETI algorithm compares favorably with leading DD methods such as the Neumann-Neumann algorithm.

We have also shown that even when the global stiffness matrix can be assembled and stored in real memory, the FETI method often outperforms optimized direct solvers on both serial and parallel/vector processors.

The FETI method has been implemented on the iPSC-860, the KSR-1, and the CM-5. It has been further extended to nonlinear time-dependent analyses and to eigenvalue problems.

### **A.2.2 Mesh Partitioning Algorithms.**

Unstructured meshes are used in several large-scale scientific and engineering problems, including finite-volume methods for computational fluid dynamics and finite element methods for structural analysis. Because of their large size and computational requirements these problems are increasingly solved on highly parallel machines and clusters of high-end workstations. If unstructured problems such as these are to be solved on distributed-memory parallel computers, their data structures must be partitioned and distributed across processors; if they are to be solved efficiently, the partitioning process must maximize load balance and minimize interprocessor communication. Recent investigations have also shown that even when computing on a parallel machine that offers a virtual shared memory environment --- such as the KSR-1 ---, mesh partitioning is still desirable because it explicitly enforces data locality and therefore ensures high levels of performance.

The development of efficient heuristics for solving the NP hard problem of graph partitioning has been a very active research area in the last few years. Under this grant, we have developed and implemented a number of fast algorithms for graph and mesh partitioning that have been demonstrated to be useful in practical large-scale computational science and engineering problems. These algorithms are: the greedy algorithm, a bandwidth minimization based algorithm, a recursive version of the latter algorithm, principal inertia algorithms and their recursive versions, a recursive graph bisection algorithm and an improved implementation of the recursive spectral bisection algorithm.

### **A.2.3 TOP/DOMDEC.**

TOP/DOMDEC is a Totally Object-oriented Program written in C++ and GL for automatic DOMain DEComposition.

It is both a software tool and a software environment for mesh partitioning and parallel processing. It is a software tool because it contains the algorithms for automatic mesh decomposition mentioned above and a set of relevant decision making tools for selecting the best mesh partition for a given problem and a given multiprocessor. It is also a software environment because it allows advanced users to "plug in" their own mesh partitioning algorithm and benefit from all the interactive features of TOP/DOMDEC that include the evaluation of load balancing, network traffic and communication costs, the generation of parallel data structures, and the use of state-of-the-art high-speed graphics. The TOP/DOMDEC project started towards the end of the funding period of this Grant but benefited from the funded development of the mesh partitioning algorithms.

#### **A.2.4 Evaluation of Parallel Hardware for Unstructured Meshes.**

We have used the algorithms and codes we have developed for parallel computations on fully unstructured grids to highlight the impact of three MPP architectures --- the CM-2, the iPSC-860, and the KSR-1 --- on the implementational strategies. On the KSR-1 system, we have contrasted two different programming approaches, one designed for fast porting and the other for high performance. We have analyzed performance results obtained on all three MPP systems in terms of interprocessor communication costs, scalability, and sheer performance. We have concluded that in general, for parallel unstructured finite element and finite volume scientific computations, a 64K CM-200 machine with a VP ratio = 1 delivers 600 real MFLOPS, a 128 processor iPSC-860 system delivers 532 real MFLOPS, and a 64 processor KSR-1 system delivers 480 MFLOPS. We have also pointed out that the KSR-1 parallel processor delivers substantially higher performance results when programmed with the local memory paradigm than with the virtual shared memory paradigm.

### **A.3 IMPACT ON COMPUTATIONAL SCIENCE INFRASTRUCTURE**

#### **A.3.1 The FETI Method.**

The FETI method has attracted the attention of several researchers in the applied mathematics and engineering fields. Professor Jan Mandel at the University of Colorado at Denver, has proved the optimal scalability of this method and has developed a dual version known as the Balancing Domain Decomposition algorithm. A team of scientists at the NASA Langley Research Center directed by Dr. Jerry Housner has also used the FETI approach to develop a procedure for the coupled analysis of independently modeled substructures. Professor Roland Keunings at the University of Louvain, Belgium, has extended its range of applications to the analysis of polymer flows.

#### **A.3.2 TOP/DOMDEC.**

The TOP/DOMDEC software for mesh partitioning and parallel processing is currently used at the NASA Ames Research Center, the NASA Lewis Research Center, the NASA Langley Research Center, the Lockheed Palo Alto Mechanics Laboratory, the Department of Electrical Engineering at the University of Michigan, the Ford Motors Research Laboratory, INRIA and ONERA in France, and the University of Liege and the University of Louvain in Belgium.

#### **A.4.1 LIST OF PUBLICATIONS IN REFEREED JOURNALS**

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2. C. Farhat and T. Y. Lin, "A Structure Attached Corotational Fluid Grid For Transient Aeroelastic Computations," AIAA Journal, Vol. 31, No. 3, pp. 597-599 (1993)
3. C. Farhat and M. Lesoinne, "Mesh Partitioning Algorithms for the Parallel Solution of P.D.E.s," Applied-Numerical Mathematics, Vol. 12, (1993)
4. C. Farhat and M. Lesoinne, "Automatic Partitioning of Unstructured Meshes for the Parallel Solution of Problems in Computational Mechanics," International Journal for Numerical Methods in Engineering, Vol. 36, No. 5, pp. 745-764 (1993)
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10. C. Farhat and F. X. Roux, "An Unconventional Domain Decomposition Method for an Efficient Parallel Solution of Large-Scale Finite Element

Systems," SIAM Journal on Scientific and Statistical Computing, Vol. 13, No. 1, pp. 379-396 (1992).

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13. C. Farhat and F. X. Roux, "A Method of Finite Element Tearing and Interconnecting and its Parallel Solution Algorithm," International Journal for Numerical Methods in Engineering, Vol. 32, pp. 1205-1227 (1991).

14. C. Farhat and E. Pramono, Mapping, "Solving and Visualizing Finite Element Problems on the Connection Machine," Parallel Processing in Engineering Applications, ed. by R. A. Adey, Computational Mechanics Publications, Springer-Verlag, pp. 95-108 (1990).

#### **A.4.2. LIST OF PUBLICATIONS IN REFEREED CONFERENCE PROCEEDINGS**

15. C. Farhat and P. S. Chen, "Regularization of the Method of Finite Element Tearing and Interconnecting," (abstract), Computational Mechanics' 92: Theory and Applications, Proceedings of the International Conference on Computational Engineering Science, Hong Kong, December 17-22, p.52 (1992).

16. C. Farhat and L. Crivelli, "Analysis and Design of Aerospace Structures on Massively Parallel Architectures: the Method of Finite Element Tearing and Interconnecting," (abstract), NASA Computational Aerosciences Conference, NASA Ames Research Center, August 18-20, pp. 118-119 (1992)

17. E. Pramono and C. Farhat, "Performance Comparison of Structural Explicit Codes on the iPSC/860 and the CM-2," (abstract), NASA Computational Aerosciences Conference, NASA Ames Research Center, August 18-20, pp. 122-123 (1992)

18. C. Farhat and F. X. Roux, "Stabilizing a Saddle-Point Domain Decomposition Method with an Augmented Lagrangian Formulation," (abstract), Proc. Sixth International Conference on Domain Decomposition Methods in Science and Engineering, p. 13 (1992).



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20. C. Farhat, "Iterative Solution of Eigenvalue Problems in Structural Dynamics Via Domain Decomposition," (abstract), Proceedings of the Copper Mountain Conference on Iterative Methods, Copper Mountain, Colorado, April 9-14 (1992).
21. C. Farhat, "Large-Scale CFD and CSM Simulations on Both Extreme Parallel Architectures: Finite Element Algorithms, Implementation Methodologies, and Performance Results," (abstract), Proceedings of the 1991 International Conference on Supercomputing, ACM Press, Cologne, Germany, June 17-21 (1991)

### **A.4.3. INTERACTIONS**

#### **Invited Presentations and Keynote Lectures**

1. NASA Computational Aerosciences Conference (CAS) on the High Performance Computing and Communications Program, NASA Ames Research Center, Moffet Field, California, August 18-20 (1992)
2. Sixth International Conference on Domain Decomposition Methods in Science and Engineering, Como, Italy, June 15-19 (1992)
3. Eighth International Conference on Vehicle Structural Mechanics and Computer Aided Engineering, Traverse City, Michigan, June 3-5 (1992) .PP
4. Fifth Copper Mountain Conference on Iterative Methods, Copper Mountain, Colorado, April 9-14 (1992)
5. 1991 International Conference on Supercomputing, Cologne, Germany, June 17-21 (1991)
6. Fifth SIAM Conference on Parallel Processing for Scientific Computing, Houston, Texas, March 25-27 (1991)
7. Parallel Methods on Large-Scale Structural Analysis and Physics Applications, NASA LaRC, Hampton, Virginia, February 5-6 (1991)

8. ICASE Workshop on Unstructured Scientific Computation on Scalable Multiprocessors, Kill Devil Hills, North Carolina, October 29-31, (1990)

9. Meeting on Domain Decomposition And Parallel Computing for Partial Differential Equations Book, ICASE, NASA LaRC, September 24-25 (1990)

**Consultative and advisory functions**

AGARD (US AIR FORCE) Consultant Mission to ONERA on Domain Decomposition Methods for Large-Scale Structural and Mechanical Problems, Paris, France, July 14-22 (1991)

## **B. ALGORITHMS AND PERFORMANCE EVALUATION OF PARALLEL MACHINES**

Oliver A. McBryan

### **B.1 PARALLEL ALGORITHMS FOR PDE SOLUTION**

The advent of massively parallel processors (MPP) initiated a search for appropriate solution algorithms for important kernels of applications. Since PDE are at the root of most scientific applications, research activity in parallel PDE algorithms has been especially intense.

There are several needs for a satisfactory parallel algorithm:

#### **Scalability:**

Scalability refers to the need for the performance of an algorithm to increase linearly with the number of processors used. Care is needed in the definition here as most algorithms are not scalable in the strict sense. Given a specific sized problem, as more processors are used the work is subdivided into smaller pieces which are usually less efficient - in the sense that communication effects between processors become increasingly important relative to computation. Thus overall performance measured as say Mflops will follow a sublinear curve as a function of numbers of process

In most application areas we are not interested in solution of a fixed size PDE that would be solvable on 1 or a few processors. The need is to solve immense problems - as large as the system will allow. Thus the more appropriate definition of scalability is that as the number of processors is increased the problem size is scaled correspondingly, and one then requires that performance scale linearly with problem size.

#### **Complexity:**

Even on a single processor, the time required to solve a problem may not scale linearly with problem size. Consider a PDE which has been discretized in terms of  $N$  degrees of freedom. The computational complexity of the algorithm refers to the dependence of solution time on  $N$ . Because very large problems of the type contemplated for solution on MPP systems will have  $N$  large and proportional to the number of processors  $P$ , algorithms whose performance does not scale approximately linearly with  $N$  will become prohibitively expensive with problem size.

The requirement for a good numerical solution method for PDE on MPP systems is then that the algorithm have computational complexity  $O(N)$  and be scalable.

### **Multigrid Methods**

Among the known scalable algorithms for elliptic PDE solution, the multigrid, domain decomposition and preconditioned conjugate gradient methods play a prominent role. In appropriate situations each has complexity close to linear in  $N$  and scales linearly in  $P$ . However multigrid methods have a particular difficulty on parallel machines in that they do not have uniform amounts of work to be performed in all phases. These algorithms use a scale of finer grids, ranging in size from 1 point to  $N$  points. When processing very coarse grids, it is impossible to effectively use  $P$  processors - for example if  $P$  is greater than the number of grid points at that level.

This inherent disadvantage of multigrid methods has led to the search for truly parallel MG methods - multigrid methods that can utilize all processors all of the time. Frederickson and McBryan developed the PSMG algorithm for this purpose. With a fine grid of size  $N$  it can utilize up to  $N$  processors all of the time. At the same time it preserves the scalability and linear complexity of standard multigrid.

### **PSMG research**

Under the current AFOSR grant we have studied many aspects of PSMG. One set of results demonstrates that the simplest PSMG algorithm is more efficient on  $N$  processors than even the fastest known conventional MG algorithms. PSMG methods are characterized by a fast convergence rate - they have a small convergence factor per iteration. While convergence rates are often used to compare methods they are not a suitable measure since the work per iteration is not considered. Therefore the normalized convergence rate is a more appropriate factor for comparison - defined as the amount of work required to reduce the error by one decimal point. For parallel algorithms one must introduce normalized convergence rates for both computation and communication and these two quantities then characterize algorithm performance. We have shown that PSMG is twice as efficient in computation and five times as efficient in communication as the optimal red-black MG algorithms - when  $N$  processors are available.

We have extended the PSMG algorithm to anisotropic equations, showing that these may be solved as easily as isotropic systems. The analysis in this case is complicated by the need to choose a semi-coarsening scheme and possibly one-dimensional solvers. The paper provides a set of measured performance data for the resulting algorithm.

## **B.2. PERFORMANCE EVALUATION OF MPP SYSTEMS**

Performance evaluation provides tools both for determining absolute performance of MPP systems as well as for relative comparison of such systems. In addition to simply measuring performance, one wants in practice to understand the measured performance. Thus performance evaluation has both an analytical and an observational aspect. We have pursued both aspects in our AFOSR research.

Performance evaluation is inherently a characteristic of the systems that are measured. We have emphasized as wide a range as possible of MPP systems - SIMD, MIMD, shared memory and distributed memory. Systems studied during this research and reported in publications include:

System	Number Nodes	Peak Mflops
Meiko CS-1	16	960
SUPRENUM-1	256	5,120
Intel iPSC2		
Intel iPSC/860	128	7,680
Thinking Machines Corp. CM-2	65536	24,000
Thinking Machines Corp. CM-200	65536	32,000
Thinking Machines Corp. CM-5	1024	131,000
Kendall Square KSR-1	64	2560
Evans and Sutherland ES-1	32	640
Myrias SP-2	128	64

Each of these systems has special characteristics that need to be understood for a proper evaluation. In fact designing appropriate performance measures is non-trivial.

We have adopted a multi-level approach to performance analysis. At the lowest level we have studied the behavior of systems in simple arithmetic and communication tasks. For example, measuring the cost of a parallel vector multiply or of a point to point data exchange. Such experiments are useful in understanding what operations actually approach the manufacturers rated peak performance, but say little about the behavior of real algorithms. At the second level we have studied the behavior of significant kernels - such as PDE solvers. These are components of full applications, but yet simple enough to be analyzed fairly completely. Typical examples that we have used include relaxation, multigrid and multi-dimensional FFT.

Our study focused on four computing systems, each representing the major parallel architecture classes: a distributed memory SIMD system (the

Connection Machine CM-2), a shared memory MIMD system (Evans & Sutherland ES-1), a shared/distributed memory hybrid system (Myrias SPS-2), and a distributed MIMD system (Intel iPSC/860). Using an integrated multilevel approach we can accurately describe the behavior of matrix/vector operations, relaxation techniques, and PDE applications on these architectures.

To demonstrate the usefulness of these models, we utilized a concrete example of a 2D fluid code describing atmospheric and oceanic systems (the Shallow Water Equations) and show how such models can predict application performance to within ten percent error.

We presented performance models of numerical computations on the Connection Machine CM-2, a massively parallel distributed memory processor array containing 65,536 processor in a hypercube topology. Our research identifies communication and computation characteristics that predict the performance of matrix/vector operations, conjugate gradient methods, relaxation techniques, and PDE applications on this architecture. Utilizing a concrete example of a 2D fluid code describing atmospheric and ocean systems, we demonstrated how such models can be used to predict application performance to within five percent error.

We studied the effectiveness of the parallel microarchitecture employed in the Intel i860 RISC microprocessor at performing matrix/vector computation kernels of scientific applications. The key issue we examined is how the data access patterns dictate system performance. We studied blocked algorithms and data mapping techniques that improve data locality of multidimensional data structures. We demonstrate that the cache miss ratio, bus utilization and external memory access optimization are the main factors driving the performance of the system.

### **B.3. Hardware Acquisition and Deployment**

AFOSR support has been critical in allowing the Center for Applied Parallel Processing (CAPP) at University of Colorado to acquire and operate a number of advanced architectures. Beginning with the acquisition of an Evans and Sutherland ES-1 in 1989, we followed with a Myrias SPS-1 in 1990 and a Kendall Square KSR-1 in 1992. These have been the ground-breaking architectures for the introduction of massively parallel shared memory approaches. We have pursued these developments because we believe that message passing approaches are so difficult from a use standpoint that they will never be widely adopted. By contrast, virtual shared memory approaches as in the Myrias SPS-1 and Kendall square KSR-1 offer the possibility of hiding all of the message passing protocol fro users. Unlike true shared memory systems, these systems are also inherently scalable.

AFOSR support was used to fund graduate research associates who become expert in the use of these systems. These students then provided consulting help to other potential users of the systems.

A second aspect of hardware integration was the development of prototype heterogeneous computing environments. A Stardent TITAN multiprocessor graphics system was acquired and was successfully interfaced to the backend of a TMC CM-2. Most of the software development involved was done by AFOSR supported graduate students. Thinking Machines Corporation was also extremely helpful in supplying software support. The resulting software was adapted by TMC as a commercial product and is currently running at many sites world-wide. The underlying concept here was to provide the ease of use of a Stardent visualization system to a Connection Machine user. Rather than implement Stardent AVS software on the CM-2, we provided an interface to CM-2 data through the high-speed CM-2 I/O ports, allowing AVS programs to be written that effectively displayed CM-2 computations in real time.

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2. O. McBryan, "Connection Machine Application Performance," in Scientific Applications of the Connection Machine,, ed. Horst Simon, pp. 94-115, World Scientific Publishing Co., Singapore, 1989.
3. O. McBryan, "Overview of Current Developments in Parallel Architectures," in Parallel Supercomputing: Methods, Algorithms and Applications, ed. G.F. Carey, pp. 17-32, John Wiley, 1989.
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7. O. McBryan, Implementation of the Shallow Water Benchmark on the SUPRENUM-1 Parallel Supercomputer, CS Dept Technical Report, University of Colorado, Boulder, 1990.

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## C. OTHER APPLICATIONS ON PARALLEL MACHINES

### C.1 COMPRESSIBLE CONVECTION AND PULSATIONS ON MASSIVELY PARALLEL COMPUTERS

Philip W. Jones

In red giant stars, convection is the dominant heat transport mechanism. This convection is vigorous and may become supersonic. Red giant stars also pulsate globally in the fundamental or first harmonic acoustic mode. Because the motions are very vigorous and the timescales for the two types of motion are similar, acoustic waves are likely to interact strongly with the convection. We have completed a series of simulations on the Connection Machine CM-2 which examine the interaction and excitation of acoustic waves with fully compressible fluid convection.

We have developed Connection Machine simulations of vigorous convection in two-dimensional polytropic models in which a layer unstable to convection is situated between two stably-stratified layers. The fully compressible fluid equations are advanced in time from this initial state using an explicit second-order Adams-Bashforth scheme for most terms, but an implicit Crank-Nicholson scheme is used for the temperature diffusion to avoid excessive restrictions on the time step. All spatial derivatives are computed using second-order finite differences. These codes are quite efficient on the CM-2, achieving scaled performances of 2.4 Gflops.

One series of simulations examined the interaction of convection with acoustic waves which were artificially driven at the lower boundary. The change in energy of the wave was analyzed by computing the work done in the frame of the wave by gas and turbulent pressures as the wave passed through the layer of fluid undergoing vigorous time-dependent convection. We found that the driving of the waves increased as a function of wave frequency and that turbulent pressure driving was comparable and even exceeded that due to gas pressure driving. Analysis of our results using a simple two-stream model of the convection indicates that wave focusing is responsible for turbulent pressure damping of the acoustic wave while driving of the waves is caused by a forced modulation due to the acoustic wave, especially where the wave amplitude is large. Red giant pulsations are large amplitude acoustic waves so the latter effects probably dominate in these stars. We also found that time-dependent convection provided a stochastic component of driving which may be responsible for irregular variability in some pulsating red giant stars.

In a second simulation, we examined supersonic penetrative convection. The convection in this case reached a Mach number of 2.4 in the upper boundary layer and exhibited a unique time-dependence, possibly due to the limited aspect ratio of our domain. This system was found to excite large amplitude acoustic waves. Such excitation has been predicted by simple models of isotropic turbulence and acoustic emissivity was predicted to increase with the cube of the Mach number. However this is the first time self-excited acoustic waves with large amplitudes have been observed in simulations of compressible convection. Based on our previous results, continued driving of this wave should be expected due to modulation of the convection by the large amplitude wave. However, our analysis is confused due to an unexpectedly strong horizontal mean component of the convective time dependence. We are currently starting another simulation with a larger aspect ratio to isolate aspect ratio effects from the wave-convection interactions.

All of the work described above was completed as part of a Ph.D. thesis which was successfully defended on 23 August 1991. At least two additional papers will be appearing soon in the *Astrophysical Journal*.

#### **C.1.1. Publications:**

1. Jones, Merryfield, and Toomre 1991, in *Challenges to Theories of the Structure of Moderate Mass Stars*, ed. J. Toomre and D. Gough, Munich: Springer-Verlag, 1991.

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### **C.2 APPLICATIONS OF MPP IN HIGH ENERGY PHYSICS**

Clive Baillie

#### **C.2.1 Spin Models**

Spin models were invented as simple statistical mechanical models of ferromagnetism. In most cases they exhibit the cooperative behavior found in phase transitions, which arises from the development of long range order in the system. The simplest example of such a model, in which the magnetic moments are assumed to be classical one-dimensional spins capable of only two orientations, is the so-called Ising model. The simplest generalization of this discrete spin model is obtained by allowing the spins to point in  $q$  directions - the  $q$ -state Potts model.

Another generalization one can make is to have continuous rather than discrete spin variables. Then the spins are represented as unit vectors in  $N$ -dimensions giving rise to the  $O(N)$  models.  $N = 1$  gives the Ising model again;  $N = 2$  is the XY model, also known as the planar Heisenberg or planar rotator model; and  $N = 3$  is the Heisenberg model.

In order to investigate the behavior of spin models near their phase transitions, Monte Carlo algorithms are traditionally used. Unfortunately the simplest algorithm -- the Metropolis algorithm -- suffers from the problem of critical slowing down, which dramatically reduces its efficiency. Therefore we use instead the new over-relaxed and cluster algorithms which help to alleviate this problem.

We have investigated the Ising,  $q=2$  Potts, XY and  $O(3)$  models in two dimensions and the Ising model in three dimensions; using various cluster algorithms.

### **C.2.2 Dynamically Triangulated Random Surfaces**

Dynamically triangulated random surfaces provide convenient discretizations of Strings that can be simulated numerically using Monte Carlo techniques. As a point particle in space moves through time it traces out a line; similarly as the string, which looks like a line in space, moves through time it sweeps out a two-dimensional surface called the worldsheet. Thus there are two ways in which to discretize the string: either the worldsheet is discretized or the ( $d$ -dimensional) space-time in which the string is embedded is discretized; we consider the former. Such discretized surface models fall into three categories: regular surfaces, fixed random surfaces and dynamical random surfaces. In the first, the surface is composed of plaquettes in a  $d$ -dimensional regular hypercubic lattice; in the second, the surface is randomly triangulated once at the beginning of the simulation; and in the third the random triangulation becomes dynamical (i.e. is changed during the simulation).

It is these dynamically triangulated random surfaces we wish to simulate. Such a simulation is, in effect, that of a fluid surface. This is because the varying triangulation means that there is no fixed reference frame, which is precisely what one would expect of a fluid where the molecules at two different points could interchange and still leave the surface intact. In string theory, this is called reparametrization invariance. Unfortunately the straight-forward simulation of such a surface yields rather disappointing results, in that the surface appears to be in a very crumpled state. The reason for this is that spike-like configurations in the surface are not suppressed, allowing it to degenerate into a spiky, crumpled object. To overcome this difficulty, one adds extrinsic curvature to smooth out the

surface. Thus we simulate dynamically triangulated random surfaces with extrinsic curvature.

An alternative way to cure the pathological nature of the surfaces is to put spin models on them. The result of this is in fact a simulation of matter coupled to quantum gravity in two dimensions. We have investigated the simplest case, namely the quenched Ising model.

### **C.2.3. Publications**

1. C. F. Baillie and P. D. Coddington, Comparison of Cluster Algorithms for two-dimensional Potts models, Phys. Rev. B43, 10617 (1991)
2. C.J. Apostolakis, C. F. Baillie, and G. C. Fox, Investigation of the 2d O(3) model using over-relaxed algorithm, Phys. Rev. D43, 2687 (1991)
3. C. F. Baillie and R. Gupta, Critical Behavior of 3D Ising and 2D XY Spin Models, Nucl. Phys. B (Proc. Suppl.) 20, 669 (1991)
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#### **D. LIST OF PERSONNEL ASSOCIATED WITH THIS RESEARCH EFFORT**

##### **D.1. Undergraduate Student:**

Bob Stoner. B. S. Computer Sciences. December 1992. Currently Software Engineer at MCI.

##### **D.2. Graduate Students**

Michel Lesoinne. Aerospace Engineering Ph.D. student; expected graduation date is May 1994.

Russ Partch. M.S. Aerospace Engineering, December 1991. Currently Ph.D. student at the Center for Space Structures and Controls, the University of Colorado at Boulder. Has been awarded the AFOSR Palace Knight Fellowship in January 1992.

Roldan Pozo, CS Dept Ph.D. student. Currently in a postdoctoral position at University of Tennessee.

Phil Jones, Astrophysics Dept Ph.D. Student. Currently a postdoc at Los Alamos National Laboratory.

Sylvia Crivelli, CS Dept MS student. Currently a Ph.D. student at CU.

Alex Reppenning, CS Dept Ph.D. student. Currently a Ph.D. student at CU.

##### **D.3. Post-Doctoral Research Assistants**

Eddy Pramono. Aerospace Engineering. Currently Research Scientist at NAS, NASA-Ames Research Center.

Luis Crivelli. Aerospace Engineering. Currently NSF fellow at the Center for Space Structures and Controls, the University of Colorado at Boulder.

Clive Baillie. Computer Science. Currently a postdoc at CU in Computer Science.